Gregory A Voth

List of Publications by Year in Descending Order

536 papers	36,352 citations	96 h-index	164 g-index
596 ext. papers	39,725 ext. citations	5.3 avg, IF	7.85 L-index

#	Paper	IF	Citations
536	Key Factors Governing Initial Stages of Lipid Droplet Formation.. *Journal of Physical Chemistry B*, **2022**, 126, 453-462	3.4	0
535	Using Machine Learning to Greatly Accelerate Path Integral Molecular Dynamics.. *Journal of Chemical Theory and Computation*, **2022**,	6.4	4
534	Cooperative multivalent receptor binding promotes exposure of the SARS-CoV-2 fusion machinery core.. *Nature Communications*, **2022**, 13, 1002	17.4	3
533	Strain and rupture of HIV-1 capsids during uncoating.. *Proceedings of the National Academy of Sciences of the United States of America*, **2022**, 119, e2117781119	11.5	2
532	Preservation of HIV-1 Gag Helical Bundle Symmetry by Bevirimat Is Central to Maturation Inhibition. *Journal of the American Chemical Society*, **2021**, 143, 19137-19148	16.4	1
531	Resolving the Structural Debate for the Hydrated Excess Proton in Water. *Journal of the American Chemical Society*, **2021**, 143, 18672-18683	16.4	5
530	Molecular interactions of the M and E integral membrane proteins of SARS-CoV-2 **2021**,		3
529	Synthesis, Characterization, and Simulation of Four-Armed Megamolecules. *Biomacromolecules*, **2021**, 22, 2363-2372	6.9	1
528	Cooperative multivalent receptor binding promotes exposure of the SARS-CoV-2 fusion machinery core **2021**,		1
527	The hopping mechanism of the hydrated excess proton and its contribution to proton diffusion in water. *Journal of Chemical Physics*, **2021**, 154, 194506	3.9	1
526	Physical Characterization of Triolein and Implications for Its Role in Lipid Droplet Biogenesis. *Journal of Physical Chemistry B*, **2021**, 125, 6874-6888	3.4	1
525	Key computational findings reveal proton transfer as driving the functional cycle in the phosphate transporter PiPT. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	3
524	Structural Characterization of Protonated Water Clusters Confined in HZSM-5 Zeolites. *Journal of the American Chemical Society*, **2021**, 143, 10203-10213	16.4	7
523	Advanced Materials for Energy-Water Systems: The Central Role of Water/Solid Interfaces in Adsorption, Reactivity, and Transport. *Chemical Reviews*, **2021**, 121, 9450-9501	68.1	9
522	A multiscale coarse-grained model of the SARS-CoV-2 virion. *Biophysical Journal*, **2021**, 120, 1097-1104	2.9	54
521	Immature HIV-1 assembles from Gag dimers leaving partial hexamers at lattice edges as potential substrates for proteolytic maturation. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	9
520	Coarse-Grained Force Fields from the Perspective of Statistical Mechanics: Better Understanding of the Origins of a MARTINI Hangover. *Journal of Chemical Theory and Computation*, **2021**, 17, 1170-1180	6.4	10

519	Molecular interactions of the´M and E integral membrane proteins of SARS-CoV-2. *Faraday Discussions*, **2021**,	3.6	5
518	Structural basis of fast- and slow-severing actin-cofilactin boundaries. *Journal of Biological Chemistry*, **2021**, 296, 100337	5.4	3
517	A new one-site coarse-grained model for water: Bottom-up many-body projected water (BUMPer). II. Temperature transferability and structural properties at low temperature. *Journal of Chemical Physics*, **2021**, 154, 044105	3.9	2
516	Lipid-Composition-Mediated Forces Can Stabilize Tubular Assemblies of I-BAR Proteins. *Biophysical Journal*, **2021**, 120, 46-54	2.9	10
515	A new one-site coarse-grained model for water: Bottom-up many-body projected water (BUMPer). I. General theory and model. *Journal of Chemical Physics*, **2021**, 154, 044104	3.9	8
514	Constructing many-body dissipative particle dynamics models of fluids from bottom-up coarse-graining. *Journal of Chemical Physics*, **2021**, 154, 084122	3.9	7
513	Compressive and Tensile Deformations Alter ATP Hydrolysis and Phosphate Release Rates in Actin Filaments. *Journal of Chemical Theory and Computation*, **2021**, 17, 1900-1913	6.4	1
512	Modeling Protein-Lipid Interactions during Viral Assembly of SARS-CoV-2. *Biophysical Journal*, **2021**, 120, 49a	2.9	78
511	Formin Cdc12's specific actin assembly properties are tailored for cytokinesis in fission yeast. *Biophysical Journal*, **2021**, 120, 2984-2997	2.9	2
510	Using Constrained Density Functional Theory to Track Proton Transfers and to Sample Their Associated Free Energy Surface. *Journal of Chemical Theory and Computation*, **2021**, 17, 5759-5765	6.4	4
509	Accurate and Transferable Reactive Molecular Dynamics Models from Constrained Density Functional Theory. *Journal of Physical Chemistry B*, **2021**, 125, 10471-10480	3.4	3
508	Integrin-based mechanosensing through conformational deformation. *Biophysical Journal*, **2021**, 120, 4349-4359	2.9	0
507	Microtubule Simulations Provide Insight into the Molecular Mechanism Underlying Dynamic Instability. *Biophysical Journal*, **2020**, 118, 2938-2951	2.9	12
506	A helical assembly of human ESCRT-I scaffolds reverse-topology membrane scission. *Nature Structural and Molecular Biology*, **2020**, 27, 570-580	17.6	19
505	What Coordinate Best Describes the Affinity of the Hydrated Excess Proton for the Air-Water Interface?. *Journal of Physical Chemistry B*, **2020**, 124, 5039-5046	3.4	2
504	Interfacial solvation and slow transport of hydrated excess protons in non-ionic reverse micelles. *Physical Chemistry Chemical Physics*, **2020**, 22, 10753-10763	3.6	2
503	TRIM5 self-assembly and compartmentalization of the HIV-1 viral capsid. *Nature Communications*, **2020**, 11, 1307	17.4	24
502	Water-Assisted Proton Transport in Confined Nanochannels. *Journal of Physical Chemistry C*, **2020**, 124, 16186-16201	3.8	6

501	Cholesterol Alters the Orientation and Activity of the Influenza Virus M2 Amphipathic Helix in the Membrane. *Journal of Physical Chemistry B*, **2020**, 124, 6738-6747	3.4	8
500	Reactive Coarse-Grained Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2020**, 16, 2541-2549	6.4	9
499	Binding mechanism of the matrix domain of HIV-1 gag on lipid membranes. *ELife*, **2020**, 9,	8.9	5
498	A Multiscale Coarse-grained Model of the SARS-CoV-2 Virion **2020**,		2
497	Temperature and Phase Transferable Bottom-up Coarse-Grained Models. *Journal of Chemical Theory and Computation*, **2020**, 16, 6823-6842	6.4	15
496	Molecular Origins of the Barriers to Proton Transport in Acidic Aqueous Solutions. *Journal of Physical Chemistry B*, **2020**, 124, 8868-8876	3.4	4
495	Multiscale Simulation Reveals Passive Proton Transport Through SERCA on the Microsecond Timescale. *Biophysical Journal*, **2020**, 119, 1033-1040	2.9	5
494	Structural basis for polarized elongation of actin filaments. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 30458-30464	11.5	6
493	Minimal Experimental Bias on the Hydrogen Bond Greatly Improves Molecular Dynamics Simulations of Water. *Journal of Chemical Theory and Computation*, **2020**, 16, 5675-5684	6.4	7
492	Density Functional Theory-Based Quantum Mechanics/Coarse-Grained Molecular Mechanics: Theory and Implementation. *Journal of Chemical Theory and Computation*, **2020**, 16, 6329-6342	6.4	4
491	Atomic-scale characterization of mature HIV-1 capsid stabilization by inositol hexakisphosphate (IP). *Science Advances*, **2020**, 6,	14.3	17
490	Influenza A M2 Inhibitor Binding Understood through Mechanisms of Excess Proton Stabilization and Channel Dynamics. *Journal of the American Chemical Society*, **2020**, 142, 17425-17433	16.4	9
489	Local conformational dynamics regulating transport properties of a Cl /H antiporter. *Journal of Computational Chemistry*, **2020**, 41, 513-519	3.5	3
488	Anisotropic Motions of Fibrils Dictated by Their Orientations in the Lamella: A Coarse-Grained Model of a Plant Cell Wall. *Journal of Physical Chemistry B*, **2020**, 124, 3527-3539	3.4	6
487	Compatible observable decompositions for coarse-grained representations of real molecular systems. *Journal of Chemical Physics*, **2019**, 151, 134115	3.9	6
486	Adversarial-residual-coarse-graining: Applying machine learning theory to systematic molecular coarse-graining. *Journal of Chemical Physics*, **2019**, 151, 124110	3.9	11
485	Systematic Coarse-Grained Lipid Force Fields with Semiexplicit Solvation via Virtual Sites. *Journal of Chemical Theory and Computation*, **2019**, 15, 2087-2100	6.4	13
484	Coarse-graining of many-body path integrals: Theory and numerical approximations. *Journal of Chemical Physics*, **2019**, 150, 244103	3.9	1

483	Off-Pathway Assembly: A Broad-Spectrum Mechanism of Action for Drugs That Undermine Controlled HIV-1 Viral Capsid Formation. *Journal of the American Chemical Society*, **2019**, 141, 10214-10224	16.4	19
482	Multiscale model of integrin adhesion assembly. *PLoS Computational Biology*, **2019**, 15, e1007077	5	12
481	Coarse-graining involving virtual sites: Centers of symmetry coarse-graining. *Journal of Chemical Physics*, **2019**, 150, 154103	3.9	9
480	Multiconfigurational Coarse-Grained Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2019**, 15, 3306-3315	6.4	13
479	Coarse-Grained Simulation of Full-Length Integrin Activation. *Biophysical Journal*, **2019**, 116, 1000-1010	2.9	9
478	Dynamic Protonation Dramatically Affects the Membrane Permeability of Drug-like Molecules. *Journal of the American Chemical Society*, **2019**, 141, 13421-13433	16.4	22
477	Plastic Deformation and Fragmentation of Strained Actin Filaments. *Biophysical Journal*, **2019**, 117, 453-463	2.9	6
476	Understanding Missing Entropy in Coarse-Grained Systems: Addressing Issues of Representability and Transferability. *Journal of Physical Chemistry Letters*, **2019**, 10, 4549-4557	6.4	25
475	Mechanical and kinetic factors drive sorting of F-actin cross-linkers on bundles. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 16192-16197	11.5	19
474	Unusual Organization of I-BAR Proteins on Tubular and Vesicular Membranes. *Biophysical Journal*, **2019**, 117, 553-562	2.9	13
473	Proton-Induced Conformational and Hydration Dynamics in the Influenza A M2 Channel. *Journal of the American Chemical Society*, **2019**, 141, 11667-11676	16.4	12
472	Ena/VASP processive elongation is modulated by avidity on actin filaments bundled by the filopodia cross-linker fascin. *Molecular Biology of the Cell*, **2019**, 30, 851-862	3.5	20
471	Lamellipodium is a myosin-independent mechanosensor. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 2646-2651	11.5	46
470	Quantum mechanics/coarse-grained molecular mechanics (QM/CG-MM). *Journal of Chemical Physics* , **2018**, 148, 014102	3.9	6
469	Multiscale Kinetic Modeling Reveals an Ensemble of Cl/H Exchange Pathways in ClC-ec1 Antiporter. *Journal of the American Chemical Society*, **2018**, 140, 1793-1804	16.4	20
468	Quantum theory of multiscale coarse-graining. *Journal of Chemical Physics*, **2018**, 148, 102335	3.9	7
467	Mechanism and Determinants of Amphipathic Helix-Containing Protein Targeting to Lipid Droplets. *Developmental Cell*, **2018**, 44, 73-86.e4	10.2	98
466	Organizing membrane-curving proteins: the emerging dynamical picture. *Current Opinion in Structural Biology*, **2018**, 51, 99-105	8.1	16

465	Ultra-Coarse-Grained Models Allow for an Accurate and Transferable Treatment of Interfacial Systems. *Journal of Chemical Theory and Computation*, **2018**, 14, 2180-2197	6.4	33
464	Mesoscopic coarse-grained representations of fluids rigorously derived from atomistic models. *Journal of Chemical Physics*, **2018**, 149, 044104	3.9	14
463	The 2018 biomembrane curvature and remodeling roadmap. *Journal Physics D: Applied Physics*, **2018**, 51,	3	133
462	Entropic forces drive clustering and spatial localization of influenza A M2 during viral budding. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, E8595-E8603	11.5	29
461	Molecular transport through membranes: Accurate permeability coefficients from multidimensional potentials of mean force and local diffusion constants. *Journal of Chemical Physics*, **2018**, 149, 072310	3.9	26
460	Simulations of N-BAR Protein Interactions with Membranes. *Journal Physics D: Applied Physics*, **2018**, 51, 35-36	3	
459	Gating mechanisms during actin filament elongation by formins. *ELife*, **2018**, 7,	8.9	14
458	Modulating the Chemical Transport Properties of a Transmembrane Antiporter via Alternative Anion Flux. *Journal of the American Chemical Society*, **2018**, 140, 16535-16543	16.4	13
457	Advances in coarse-grained modeling of macromolecular complexes. *Current Opinion in Structural Biology*, **2018**, 52, 119-126	8.1	60
456	Ultra-Coarse-Grained Liquid State Models with Implicit Hydrogen Bonding. *Journal of Chemical Theory and Computation*, **2018**, 14, 6159-6174	6.4	10
455	Multiscale simulation of actin filaments and actin-associated proteins. *Biophysical Reviews*, **2018**, 10, 1521-1535	3.7	4
454	Insights into the Cooperative Nature of ATP Hydrolysis in Actin Filaments. *Biophysical Journal*, **2018**, 115, 1589-1602	2.9	20
453	The Theory of Ultra-Coarse-Graining. 3. Coarse-Grained Sites with Rapid Local Equilibrium of Internal States. *Journal of Chemical Theory and Computation*, **2017**, 13, 1010-1022	6.4	39
452	Highly Coarse-Grained Representations of Transmembrane Proteins. *Journal of Chemical Theory and Computation*, **2017**, 13, 935-944	6.4	11
451	Communication: Improved ab initio molecular dynamics by minimally biasing with experimental data. *Journal of Chemical Physics*, **2017**, 146, 041102	3.9	17
450	IR spectral assignments for the hydrated excess proton in liquid water. *Journal of Chemical Physics*, **2017**, 146, 154507	3.9	52
449	Reactive molecular dynamics models from molecular dynamics data using relative entropy minimization. *Chemical Physics Letters*, **2017**, 683, 573-578	2.5	3
448	Non-uniqueness of quantum transition state theory and general dividing surfaces in the path integral space. *Journal of Chemical Physics*, **2017**, 146, 174106	3.9	4

447	Friction Mediates Scission of Tubular Membranes Scaffolded by BAR Proteins. *Cell*, **2017**, 170, 172-184.e11	36.2	128
446	Role of solvation structure in the shuttling of the hydrated excess proton. *Journal of Chemical Sciences*, **2017**, 129, 1045-1051	1.8	3
445	Understanding the essential proton-pumping kinetic gates and decoupling mutations in cytochrome oxidase. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 5924-5929	11.5	24
444	Simulating Protein Mediated Hydrolysis of ATP and Other Nucleoside Triphosphates by Combining QM/MM Molecular Dynamics with Advances in Metadynamics. *Journal of Chemical Theory and Computation*, **2017**, 13, 2332-2341	6.4	25
443	A Multiscale Description of Biomolecular Active Matter: The Chemistry Underlying Many Life Processes. *Accounts of Chemical Research*, **2017**, 50, 594-598	24.3	13
442	Mechanoregulated inhibition of formin facilitates contractile actomyosin ring assembly. *Nature Communications*, **2017**, 8, 703	17.4	44
441	Phosphomimetic S3D cofilin binds but only weakly severs actin filaments. *Journal of Biological Chemistry*, **2017**, 292, 19565-19579	5.4	20
440	Delocalization and stretch-bend mixing of the HOH bend in liquid water. *Journal of Chemical Physics* , **2017**, 147, 084503	3.9	38
439	The mesoscopic membrane with proteins (MesM-P) model. *Journal of Chemical Physics*, **2017**, 147, 044104	3.9	14
438	Actin Filament Strain Promotes Severing and Cofilin Dissociation. *Biophysical Journal*, **2017**, 112, 2624-2633	2.9	30
437	Extending the range and physical accuracy of coarse-grained models: Order parameter dependent interactions. *Journal of Chemical Physics*, **2017**, 147, 044113	3.9	38
436	Coarse-Grained Directed Simulation. *Journal of Chemical Theory and Computation*, **2017**, 13, 4593-4603	6.4	10
435	Development of reactive force fields using ab initio molecular dynamics simulation minimally biased to experimental data. *Journal of Chemical Physics*, **2017**, 147, 161719	3.9	11
434	Long-Range Organization of Membrane-Curving Proteins. *ACS Central Science*, **2017**, 3, 1246-1253	16.8	18
433	Proton movement and coupling in the POT family of peptide transporters. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 13182-13187	11.5	38
432	Immature HIV-1 lattice assembly dynamics are regulated by scaffolding from nucleic acid and the plasma membrane. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E10056-E10065	11.5	40
431	Competition between Tropomyosin, Fimbrin, and ADF/Cofilin drives their sorting to distinct actin filament networks. *ELife*, **2017**, 6,	8.9	50
430	Acid activation mechanism of the influenza A M2 proton channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E6955-E6964	11.5	51

429	The Origin of Coupled Chloride and Proton Transport in a Cl/H Antiporter. *Journal of the American Chemical Society*, **2016**, 138, 14923-14930	16.4	29
428	Coarse-grained simulation reveals key features of HIV-1 capsid self-assembly. *Nature Communications*, **2016**, 7, 11568	17.4	85
427	Multiscale simulations reveal key features of the proton-pumping mechanism in cytochrome c oxidase. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 7420-5	11.5	37
426	Multiscale simulations of protein-facilitated membrane remodeling. *Journal of Structural Biology*, **2016**, 196, 57-63	3.4	13
425	The F-actin bundler □actinin Ain1 is tailored for ring assembly and constriction during cytokinesis in fission yeast. *Molecular Biology of the Cell*, **2016**, 27, 1821-33	3.5	35
424	Role of Presolvation and Anharmonicity in Aqueous Phase Hydrated Proton Solvation and Transport. *Journal of Physical Chemistry B*, **2016**, 120, 1793-804	3.4	51
423	Cations Stiffen Actin Filaments by Adhering a Key Structural Element to Adjacent Subunits. *Journal of Physical Chemistry B*, **2016**, 120, 4558-67	3.4	25
422	Hydroxide Solvation and Transport in Anion Exchange Membranes. *Journal of the American Chemical Society*, **2016**, 138, 991-1000	16.4	155
421	Proton Solvation and Transport in Realistic Proton Exchange Membrane Morphologies. *Journal of Physical Chemistry C*, **2016**, 120, 3176-3186	3.8	33
420	Computationally Efficient Multiscale Reactive Molecular Dynamics to Describe Amino Acid Deprotonation in Proteins. *Journal of Chemical Theory and Computation*, **2016**, 12, 879-91	6.4	32
419	Molecular modeling and assignment of IR spectra of the hydrated excess proton in isotopically dilute water. *Journal of Chemical Physics*, **2016**, 145, 154504	3.9	17
418	Dynamic force matching: Construction of dynamic coarse-grained models with realistic short time dynamics and accurate long time dynamics. *Journal of Chemical Physics*, **2016**, 145, 224107	3.9	23
417	Can quantum transition state theory be defined as an exact t = 0+ limit?. *Journal of Chemical Physics* , **2016**, 144, 084110	3.9	5
416	On the representability problem and the physical meaning of coarse-grained models. *Journal of Chemical Physics*, **2016**, 145, 044108	3.9	72
415	Multiscale Simulations Reveal Key Aspects of the Proton Transport Mechanism in the ClC-ec1 Antiporter. *Biophysical Journal*, **2016**, 110, 1334-45	2.9	37
414	Coupling Protein Dynamics with Proton Transport in Human Carbonic Anhydrase II. *Journal of Physical Chemistry B*, **2016**, 120, 8389-404	3.4	21
413	A Direct Method for Incorporating Experimental Data into Multiscale Coarse-Grained Models. *Journal of Chemical Theory and Computation*, **2016**, 12, 2144-53	6.4	22
412	Transition-Tempered Metadynamics Is a Promising Tool for Studying the Permeation of Drug-like Molecules through Membranes. *Journal of Chemical Theory and Computation*, **2016**, 12, 5157-5169	6.4	33

411	Fascin- and α-Actinin-Bundled Networks Contain Intrinsic Structural Features that Drive Protein Sorting. *Current Biology*, **2016**, 26, 2697-2706	6.3	58
410	How curvature-generating proteins build scaffolds on membrane nanotubes. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 11226-11231	11.5	91
409	An analysis of hydrated proton diffusion in ab initio molecular dynamics. *Journal of Chemical Physics* , **2015**, 142, 014104	3.9	50
408	Hydrated Proton Structure and Diffusion at Platinum Surfaces. *Journal of Physical Chemistry C*, **2015** , 119, 14675-14682	3.8	10
407	Predicting the Sensitivity of Multiscale Coarse-Grained Models to their Underlying Fine-Grained Model Parameters. *Journal of Chemical Theory and Computation*, **2015**, 11, 3547-60	6.4	10
406	Designing free energy surfaces that match experimental data with metadynamics. *Journal of Chemical Theory and Computation*, **2015**, 11, 2451-60	6.4	42
405	Propensity of Hydrated Excess Protons and Hydroxide Anions for the Air-Water Interface. *Journal of the American Chemical Society*, **2015**, 137, 12610-6	16.4	78
404	When Physics Takes Over: BAR Proteins and Membrane Curvature. *Trends in Cell Biology*, **2015**, 25, 780-792	12.3	183
403	Exploring Valleys without Climbing Every Peak: More Efficient and Forgiving Metabasin Metadynamics via Robust On-the-Fly Bias Domain Restriction. *Journal of Chemical Theory and Computation*, **2015**, 11, 5638-50	6.4	23
402	Dynamic force matching: A method for constructing dynamical coarse-grained models with realistic time dependence. *Journal of Chemical Physics*, **2015**, 142, 154104	3.9	64
401	Ion mixing, hydration, and transport in aqueous ionic systems. *Journal of Chemical Physics*, **2015**, 142, 184905	3.9	13
400	A reductionist perspective on quantum statistical mechanics: Coarse-graining of path integrals. *Journal of Chemical Physics*, **2015**, 143, 094104	3.9	7
399	The multiscale coarse-graining method. XI. Accurate interactions based on the centers of charge of coarse-grained sites. *Journal of Chemical Physics*, **2015**, 143, 243116	3.9	24
398	Membrane tension controls the assembly of curvature-generating proteins. *Nature Communications* , **2015**, 6, 7219	17.4	119
397	Mesoscale Study of Proton Transport in Proton Exchange Membranes: Role of Morphology. *Journal of Physical Chemistry C*, **2015**, 119, 1753-1762	3.8	28
396	Ion Transport through Ultrathin Electrolyte under Applied Voltages. *Journal of Physical Chemistry B*, **2015**, 119, 7516-21	3.4	12
395	Hydrated Excess Protons Can Create Their Own Water Wires. *Journal of Physical Chemistry B*, **2015**, 119, 9212-8	3.4	60
394	Electrostatic interactions between the Bni1p Formin FH2 domain and actin influence actin filament nucleation. *Structure*, **2015**, 23, 68-79	5.2	12

393	Highly Scalable and Memory Efficient Ultra-Coarse-Grained Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 423-31	6.4	22
392	Persistent Subdiffusive Proton Transport in Perfluorosulfonic Acid Membranes. *Journal of Physical Chemistry Letters*, **2014**, 5, 3037-42	6.4	27
391	Special Issue on Free Energy. *Journal of Chemical Theory and Computation*, **2014**, 10, 2631	6.4	3
390	Well-tempered metadynamics converges asymptotically. *Physical Review Letters*, **2014**, 112, 240602	7.4	182
389	Proton transport under external applied voltage. *Journal of Physical Chemistry B*, **2014**, 118, 8090-8	3.4	18
388	Interactions of protein kinase C-□C1A and C1B domains with membranes: a combined computational and experimental study. *Journal of the American Chemical Society*, **2014**, 136, 11757-66	16.4	26
387	Benchmark Study of the SCC-DFTB Approach for a Biomolecular Proton Channel. *Journal of Chemical Theory and Computation*, **2014**, 10, 451-462	6.4	27
386	Chloride Enhances Fluoride Mobility in Anion Exchange Membrane/Polycationic Systems. *Journal of Physical Chemistry C*, **2014**, 118, 845-853	3.8	21
385	Insights into the transport of aqueous quaternary ammonium cations: a combined experimental and computational study. *Journal of Physical Chemistry B*, **2014**, 118, 1363-72	3.4	22
384	Unraveling the mystery of ATP hydrolysis in actin filaments. *Journal of the American Chemical Society*, **2014**, 136, 13053-8	16.4	51
383	Transition-Tempered Metadynamics: Robust, Convergent Metadynamics via On-the-Fly Transition Barrier Estimation. *Journal of Chemical Theory and Computation*, **2014**, 10, 3626-33	6.4	47
382	Nucleotide regulation of the structure and dynamics of G-actin. *Biophysical Journal*, **2014**, 106, 1710-20	2.9	16
381	Path Integral Coarse-Graining Replica Exchange Method for Enhanced Sampling. *Journal of Chemical Theory and Computation*, **2014**, 10, 3634-40	6.4	9
380	Efficient and Minimal Method to Bias Molecular Simulations with Experimental Data. *Journal of Chemical Theory and Computation*, **2014**, 10, 3023-30	6.4	63
379	Proton Transport Mechanism of Perfluorosulfonic Acid Membranes. *Journal of Physical Chemistry C*, **2014**, 118, 17436-17445	3.8	63
378	Multiscale simulation reveals a multifaceted mechanism of proton permeation through the influenza A M2 proton channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 9396-401	11.5	60
377	An Electrochemically and Thermally Switchable Donor□Acceptor [c2]Daisy Chain Rotaxane. *Angewandte Chemie*, **2014**, 126, 1984-1989	3.6	16
376	Electron transfer activation of a second water channel for proton transport in [FeFe]-hydrogenase. *Journal of Chemical Physics*, **2014**, 141, 22D527	3.9	13

375	Solvent-Free, Highly Coarse-Grained Models for Charged Lipid Systems. *Journal of Chemical Theory and Computation*, **2014**, 10, 4730-4744	6.4	18
374	Can the ring polymer molecular dynamics method be interpreted as real time quantum dynamics?. *Journal of Chemical Physics*, **2014**, 140, 154103	3.9	22
373	The Theory of Ultra-Coarse-Graining. 2. Numerical Implementation. *Journal of Chemical Theory and Computation*, **2014**, 10, 5265-75	6.4	49
372	Nucleotide-dependent lateral and longitudinal interactions in microtubules. *Journal of Molecular Biology*, **2013**, 425, 2232-46	6.5	25
371	Molecular mechanism of membrane binding of the GRP1 PH domain. *Journal of Molecular Biology*, **2013**, 425, 3073-90	6.5	46
370	Understanding the role of amphipathic helices in N-BAR domain driven membrane remodeling. *Biophysical Journal*, **2013**, 104, 404-11	2.9	73
369	Effects of ATP and actin-filament binding on the dynamics of the myosin II S1 domain. *Biophysical Journal*, **2013**, 105, 1624-34	2.9	12
368	On the origin of proton mobility suppression in aqueous solutions of amphiphiles. *Journal of Physical Chemistry B*, **2013**, 117, 15426-35	3.4	9
367	Molecular Dynamics Simulations of Proton Transport in 3M and Nafion Perfluorosulfonic Acid Membranes. *Journal of Physical Chemistry C*, **2013**, 117, 8079-8091	3.8	77
366	Linear aggregation of proteins on the membrane as a prelude to membrane remodeling. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 20396-401	11.5	119
365	Protein-mediated transformation of lipid vesicles into tubular networks. *Biophysical Journal*, **2013**, 105, 711-9	2.9	68
364	Discovering crystals using shape matching and machine learning. *Soft Matter*, **2013**, 9, 8552	3.6	32
363	Exploring the behaviour of the hydrated excess proton at hydrophobic interfaces. *Faraday Discussions*, **2013**, 167, 263-78	3.6	30
362	A Hybrid Approach for Highly Coarse-grained Lipid Bilayer Models. *Journal of Chemical Theory and Computation*, **2013**, 9, 750-765	6.4	56
361	Coarse-graining of proteins based on elastic network models. *Chemical Physics*, **2013**, 422, 165-174	2.3	22
360	Autoinhibition of endophilin in solution via interdomain interactions. *Biophysical Journal*, **2013**, 104, 396-403	2.9	18
359	Molecular origins of cofilin-linked changes in actin filament mechanics. *Journal of Molecular Biology*, **2013**, 425, 1225-40	6.5	36
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